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THE RIEMANN PROBLEM FOR A MODEL NON-LINEAR ELASTIC CONTINUUM

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The solution to the Riemann problem for a non-linear elastic continuum characterized by an internal energy density $\epsilon(S, \epsilon_{ij})$, where S is the entropy and ϵ_{ij} the strain tensor, is discussed. Numerical solutions for the wave structure for parameters appropriate to Tungsten are discussed.

1 INTRODUCTION

The integration of the equations of Lagrangian hydrodynamics of fluids and continua requires the solution of a Riemann problem when the schemes of Glimm or Godunov are used.[1] This problem has typically been studied for fluid equations of state.[2] When elastic continua are studied, the lower symmetry and consequent increase in the dimensionality of the space of dynamical variables introduce complications.[3] In the following we present a model internal energy appropriate for large density changes and discuss the numerical solution to the Riemann initial value problem. Section 2 describes the Riemann problem. Section 3 describes the model. Section 4 describes a scheme for solution and Section 5 discusses some numerical results.

2 THE RIEMANN PROBLEM FOR AN ELASTIC CONTINUUM

The conservation laws for a non linear elastic continuum give rise to a set of quasi linear hyperbolic equations

$$\rho \partial_t v_i - a_{ik}^{-1} \partial_k \sigma_{ij} = 0 \tag{1}$$

$$\rho \partial_t E - a_{kj}^{-1} \partial_k (v_i \sigma_{ij}) = 0 \tag{2}$$

$$\partial_t a_{ij} - \partial_j v_i = 0 \tag{3}$$

In writing these we assume a Lagrangian representation with X the Lagrangian coordinate defined in the usual way

$$x_i = X_i + u_i(\vec{X}, t), \tag{4}$$

$$X_i = x_i(\vec{X}, t = 0) \tag{5}$$

The velocity of a material element $\vec{v}$, the deformation tensor a and the Cauchy stress tensor σ are then given by

$$v_i = \left.\frac{\partial x_i}{\partial t}\right|_X = \left.\frac{\partial u_i}{\partial t}\right|_X \equiv \partial_t u_i, \tag{6}$$

$$a_{ij} = \left.\frac{\partial x_i}{\partial X_j}\right|_t \equiv \partial_j x_i, \tag{7}$$

$$\sigma_{ij} = \rho \left.\frac{\partial \epsilon}{\partial a_{ij}}\right|_S, \tag{8}$$

where σ is the stress tensor. The specific internal energy ϵ is related to the total energy E by

$$E = \epsilon + \frac{1}{2} v^2 \tag{9}$$

In the above we assume local thermodynamic equilibrium so that the local internal energy is a function of the entropy and strain tensor.

In the Riemann problem which will be considered here we assume a flow depending only on X_1 and t

Then only X_1, derivatives are relevant. We may define vector stresses and strains

$$s_i \equiv \sigma_{i1}, \tag{10}$$

$$p_i \equiv \partial_1 v_i. \tag{11}$$

The conservation equations may then be written as

$$\partial_t u + \partial_1 f = 0, \tag{12}$$

where u and f are the seven dimensional vectors

$$u \equiv [\vec{v}, \vec{p}, \rho_o E], \tag{13}$$

$$f \equiv \left[-\frac{1}{\rho_o}\vec{s}, -\vec{v}, -(\vec{v}\cdot\vec{s}) \right], \tag{14}$$

and ρ_o is the Lagrangian density

$$\rho = \frac{\rho_o}{1+p_1}. \tag{15}$$

In this representation the first law of thermodynamics reads

$$\rho_o de = \rho_o T dS + s_i dp_i. \tag{16}$$

The solution to the Riemann problem is defined to be the self similar solution of equations (12) for the initial condition

$$u(t=0) = \begin{cases} u(1) & (X_1 < 0) \\ u(2) & (X_1 > 0) \end{cases} \tag{17}$$

where $u(1)$ and $u(2)$ are constant vectors.

3 A MODEL EQUATION OF STATE

The specific internal energy depends on the specific entropy and the strain tensor. The adiabatic elastic constants are formed by taking constant entropy strain derivatives of this quantity. In situations involving strong variations of the local thermodynamic variables it is important to include the strain dependence of these quantities. These variations are calculable in principle, at least for the simple metals for which pseudo potential theories give reasonably accurate representations of the shape dependence of the free energy and reasonable representations of the electronic and phononic contributions to the entropy. However, since we are interested here in numerical questions related to the solutions of (12) and (17), we prefer to use a reasonably simple yet accurate model internal energy.

We write the stress as a sum of a cold stress and a thermal stress

$$s_i(\vec{p}, e) = s_i^{(o)}(\vec{p}) + \delta s_i(\vec{p}, e), \tag{18}$$

$$e_{th}(\vec{p}, e) = \rho_o \gamma_i(\vec{p}, e)[e - e^{(o)}(\vec{p})], \tag{19}$$

where γ_i are Grüneisen functions and $e^{(o)}(\vec{p})$ is the cold energy. A reasonable approximation to the cold equation of state approximates the bulk modulus as a constant plus a term linear in the pressure. This results in an elastic constant of the form

$$\mu_1(p_1) = \frac{\mu_1(0)}{(1+p_1)}\left(\frac{\rho}{\rho(0)}\right)^{\Gamma_1}, \tag{20}$$

with $\rho(0)$ a reference density. We make a minimal assumption that the transverse elastic constants depend only on the density with the form (20).

The elastic constants satisfy general symmetry requirements as is well known. In the Lagrangian formulation it is possible to show that

$$\frac{\partial s_i}{\partial p_{1,j}} = \frac{\partial s_j}{\partial p_{1,i}}. \tag{21}$$

Since this relationship is satisfied a fortiori by the cold stress it follows from the definition of δs that

$$\frac{\partial \gamma_i}{\partial p_j}\Big|_S = \frac{\partial \gamma_j}{\partial p_i}\Big|_S \tag{22}$$

The assumption that the cold transverse elastic constants depend only on p_1, viz.

$$s_2^{(e)}(\vec{p}) \equiv \nu_2(p_1)(p_2 - p_2(o)), \tag{23}$$

$$s_3^{(e)}(\vec{p}) \equiv \nu_3(p_1)(p_3 - p_3(o)), \tag{24}$$

with

$$\nu_i(p_1) = \frac{\mu_i(o)}{(1+p_1)}\left(\frac{\rho}{\rho(o)}\right)^{\Gamma_i}, \tag{25}$$

requires in view of eqn (21) that $s_1^{(e)}(\vec{p})$, depend on p_2 and p_3 as well. Since this information is not generally available (although in principle calculable) we modify $s_1^{(e)}(\vec{p})$ by including a quadratic term so that (21) is satisfied. Similar remarks apply for the γ_i which we write as

$$\gamma_1(\vec{p}) = \left(\frac{\rho}{\rho_o}\right)\gamma_1(o) + \frac{1}{2}\left(\frac{\rho}{\rho_o}\right)^2 \gamma_2(o)(p_2 - p_2(o))^2 + \frac{1}{2}\left(\frac{\rho}{\rho_o}\right)^2 \gamma_3(o)(p_3 - p_3(o))^2 \tag{26}$$

$$\gamma_2(\vec{p}) = \left(\frac{\rho}{\rho_o}\right)\gamma_2(o)(p_2 - p_2(o)), \tag{27}$$

$$\gamma_3(\vec{p}) = \left(\frac{\rho}{\rho_o}\right)\gamma_3(o)(p_3 - p_3(o)) \tag{28}$$

The minimal set of parameters are then $\mu_i(o)$, $\gamma_i(o)$ and Γ_i, nine in all.

4 NUMERICAL METHODS

We denote the regions of constant u separated by discontinuities as (1 1), (1 2), (1 3), (2 3), (2 2), (2 1) where (1 1) is the left most state and (2 1) the right most state. Following Lax[4] we write the constant solutions in regions (1 3) and (2 3) as three parameter functions of the initial states

$$u(1,3) = F(u(1); \eta_{11}, \eta_{12}, \eta_{13}), \tag{29}$$

$$u(2,3) = F(u(2); \eta_{21}, \eta_{22}, \eta_{23}). \tag{30}$$

The conditions of solution are the requirements that

$$v_1(2,3) - v_1(1,3) = 0, \tag{31}$$

$$s_1(2,3) - s_1(1,3) = 0. \tag{32}$$

i.e. that the velocities and stresses are continuous across the contact discontinuity. This amounts to a six dimensional nonlinear function solve in the η_{ij} space. To test the feasibility of such a solution method we have considered the situation for which it is a reasonable approximation to replace isentropes with Hugoniot curves. Then the function F in (29) and (30) is determined by the Rankine Hugoniot conditions. We have found that p_1 is a good choice for the parameter η_{ij}.

The linearization of the above procedure results in an eigenvalue problem of the form

$$\Delta p_1(k,j) = M_{kj}^{-1} v_j \tag{33}$$

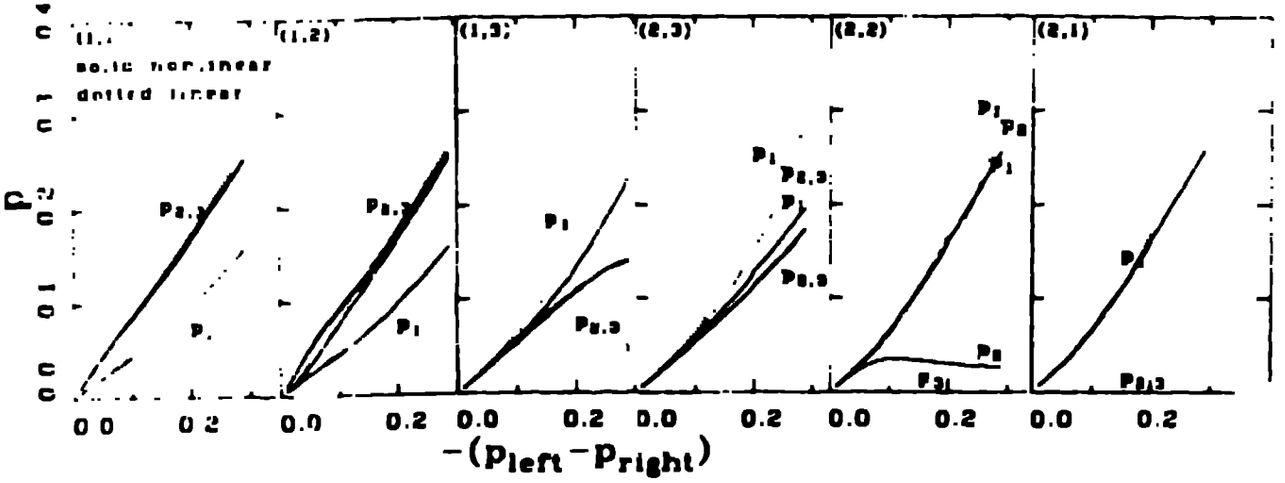
where M is a constant matrix depending on the left and right states 1 and 2, v is the vector

$$v = (v(2) - v(1), s(2) - s(1)), \tag{34}$$

and Δp_1 is the change of p_1 across a discontinuity and determines the parameter $\eta_{kj} = p_1(k,j)$. The full problem, however, requires a nonlinear solution and our procedure has been to write

$$u(1,o) = u(1), \quad u(1,n+1) = u(2), \quad u(2,n+1) = u(2),$$

and iterate from $n = 1$ to $n = I$



5 DISCUSSION

The detailed description of numerical results will be presented in a longer report. A typical example is a Tungsten like model for which we have taken $\mu_1(o) = 3.18$ Mbar, $\mu_2(o) = 1.64$ Mbar, $\mu_3(o) = 1.54$ Mbar, $\gamma_1(o) = 1.78$, $\gamma_2(o) = \gamma_3(o) = 1.78$, $\Gamma_1 = 4.00$, $\Gamma_2 = \Gamma_3 = 3.00$. Initial values have been chosen to be $v_s(1) - v_s(2) = 0$, $p_s(2) = 10^{-6}$, $\rho_o e_{th}(1) = 10^{-5}$ Mbar, $\rho_o e_{th}(2) = 10^{-6}$ Mbar where $e_{th} = e - e_{cold}$ is the thermal energy, and $p_s(1) \equiv p$ has been varied. The strains in the different regions as a function of p are shown in the figure. One result which is apparent from these calculations is that for a range $|\vec{s}| < \frac{1}{4}\mu_1(o)$, the linear state vectors are rather good approximations to the actual solutions (differing by the order of 10 per cent at the upper end). Beyond this range non linearity becomes important. Indeed, for $|\vec{s}| \approx 2\mu_1(o)$, in this model, the eigenvalues of the matrix M become imaginary. The above suggests that a perturbative approach may be useful. However such an approach has not been pursued.

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